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Fachbereich C – Mathematik und Naturwissenschaften
Angewandte Mathematik / Numerische Analysis

Numerical Analysis and Simulation I: Ordinary Differential Equations (ODEs)

Sheet 1 - ODE Models in Science

Return of the Exercise Sheet: Tuesday, October 28th before the lecture

Exercise 1: *Epidemic model for HIV Infection in a Homosexual Population*
An early model for the development of an AIDS epidemic in a homosexual population is due to Anderson et al. (1986). Though much less specific and less directly related to current HIV thinking, it is an instructive example for constructing an epidemic model using a chart flow.

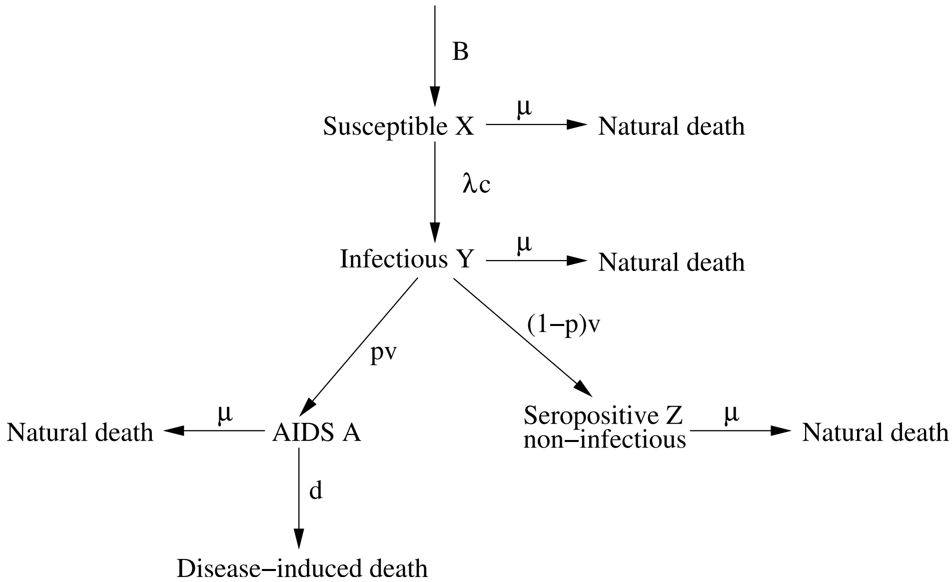


Figure 1: B represents the recruitment of susceptible into the homosexual community.
The rate of transferal from the susceptible to the infectious class is λc, where λ is the probability of acquiring infection from a randomly chosen partner and c is the number of sexual partners. A proportion of the infectious class is assumed to become noninfectious with rest developing AIDS. Natural (non-AIDS induced) death is also included in the model.

Let us assume there is a constant immigration rate B of susceptible males (susceptible $\equiv$ can catch the disease) into a population of size $N(t) = X(t) + Y(t) + A(t) + Z(t)$. Let $X(t), Y(t), A(t)$ and $Z(t)$ denote respectively the number of susceptible, infectious males, AIDS patients and the number of HIV-positive or seropositive men who are non infectious. We assume susceptibles die naturally at a rate μ. We assume AIDS patients die at a rate d: $1/d$ is of the order of months to years, more often the latter. Our model is based on the flow diagram of the disease shown in the figure above.
Here, μ is the natural (non-AIDS related) death rate, λ is the probability of acquiring infection from a randomly chosen partner ($\lambda = \beta Y/(X+Y+Z) \approx \beta Y/N$ — A is considered small in comparison with N —, where β is the transmission probability), c is the number of sexual partners, d is the AIDS-related death rate, p is the proportion of HIV-positive who are infectious and v is the rate of conversion from infection to AIDS here to be taken constant. $1/v$ is then the average incubation time of the disease.
Formulate a reasonable first model system based on the flow diagram in the figure above, i.e. determine differential equations for X, Y, A and Z, e.g.

$$\dot{X} = B - \mu X - \lambda c X, \quad \lambda = \frac{\beta Y}{N}.$$

Exercise 2: *Ozone decay*
The process of ozone decay that takes place in the atmosphere is described by the chemical reactions

$$\begin{aligned} O_3 + O_2 &\xrightarrow{k_1} O + 2O_2, \\ O + 2O_2 &\xrightarrow{k_2} O_3 + O_2, \\ O_3 + O &\xrightarrow{k_3} 2O_2, \end{aligned}$$

with reaction rate coefficients $k_1, k_2, k_3 > 0$.
Set up the corresponding system of ordinary differential equations for the three unknown concentrations $y_1 = c_{O_3} = [O_3],\ y_2 = c_O = [O],\ y_3 = c_{O_2} = [O_2]$.

Homework 1: *Law of mass action* (10 Points)
A bimolecular chemical reaction and its reverse reaction is given by

$$A \; + \; B \; \underset{k_2}{\overset{k_1}{\rightleftharpoons}} \; C \; + \; D$$

with the velocities $k_1, k_2 > 0$. Let $c_S(t)$ be the concentration of the molecule S at time t.

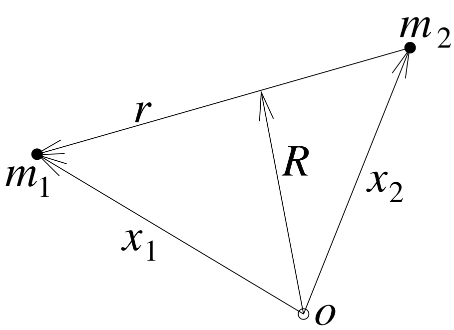
a) Formulate a system of ordinary differential equations for the unknowns $y_1 = c_A,\ y_2 = c_B,\ y_3 = c_C,\ y_4 = c_D$.
Hint: The bimolecular reaction can be re-written by the reactions

$$\begin{aligned} & A + B \xrightarrow{k_1} C + D \\ \textit{and}\quad & C + D \xrightarrow{k_2} A + B \end{aligned}$$

b) An equilibrium is given if $y_i' = 0$ holds for all $i = 1, 2, 3, 4$. Use this condition to derive the law of mass action, i.e., determine the ratio k_1/k_2 in dependence on the concentrations in equilibrium.

Homework 2: *Two-body problem* (10 Points)
The two-body problem with masses $m_1, m_2 > 0$ implies a system of ODEs for $\vec{x}_1''$ and $\vec{x}_2''$. Now new variables are introduced: $\vec{R}$ corresponds to the center of gravity, whereas $\vec{r}$ represents the relative position of the masses:

$$\begin{aligned} \vec{R} &= \frac{m_1\vec{x}_1 + m_2\vec{x}_2}{m_1 + m_2}, \\ \vec{r} &= \vec{x}_1 - \vec{x}_2. \end{aligned}$$



Arrange a system of ODEs for $\vec{R}''$ and $\vec{r}''$. Perform an interpretation of this system and its solution.